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Towards soil property retrieval from space: A one-dimensional twin-experiment

Ranmalee Bandara *, Jeffrey P. Walker, Christoph Rüdiger

Department of Civil Engineering, Monash University, Clayton 3800, Australia

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S U M M A R Y

Soil moisture is among the key environmental variables controlling evaporation, infiltration and runoff. However, the temporal evolution of soil moisture is not easy to measure or monitor at large scales due to its spatial variability, which is largely driven by local variation in soil properties and vegetation cover. Consequently, soil moisture estimates using land surface models are typically made using effective physical parameterisations based on low-resolution and/or erroneous soil property information. Thus, land surface models have an urgent need for more accurate and detailed soil parameter data sets than are currently available, in order to undertake regional or global simulation studies at high spatial resolution and with the required accuracy. To overcome this limitation, the possibility of estimating the soil hydraulic properties through model calibration to remotely sensed near-surface soil moisture observation is explored. The study presents a methodology that demonstrates this potential using a synthetic twin experiment framework, thus avoiding the need to deal with possible model-observation biases. Moreover, it explores a range of scenarios, with the objective to determine the best meteorologic conditions for soil property retrieval and hence the most efficient use of computational resources when applying the methodology at large scales. These scenarios include: (a) short dry-down period, (b) short dry period, (c) short wet-up period, (d) short wet period and (e) full 12-months with multiple wetting and drying periods. The methodology was also tested for four different soil types including a homogeneous column of sand, a homogeneous column of clay, a duplex column of clay over sand, and a duplex column of silty sand over clay. The study showed that soil hydraulic parameters were best retrieved when using the full 12-month period, with the sequential retrieval of three parameters at a time being the most suitable approach when retrieving the six parameters, with the most sensitive parameters retrieved first.

1. Introduction

The moisture content of the soil is a key variable controlling the exchange of water and energy fluxes between the land surface and the atmosphere, as it affects the evaporation and plant transpiration. Hence the soil moisture is an important contributor to the development of weather patterns including precipitation (Dirmeyer et al., 2009; Koster et al., 2004) and air temperature (Timbal et al., 2001). Indeed, soil moisture plays an essential role in most environmental processes (Seneviratne et al., 2010), and is one of the few important hydrological variables that is directly observable. Moreover, it has been declared an Essential Climate Variable by the Global Climate Observing System (GCOS) (Stitt et al., 2011), and is therefore a reportable land surface parameter for the contributing members. However, the temporal evolution of high-resolution soil moisture is not straight forward to monitor across large scales, both from a logistical and an economic point of view, due to its high spatial variability. Both active and passive remote sensing methods are being utilized in soil moisture monitoring, including the Advanced Microwave Scanning Radiometer for Earth Observation System (AMSR-E; C- and X-band) (Njoku and Li, 1997; Owe et al., 2008), Advanced Scatterometer (ASCAT; C-band) (Albergel et al., 2009) and Soil Moisture and Ocean Salinity (SMOS; L-band) (Kerr et al., 2010). However, remote sensing techniques only provide information on the near surface layer of soil, and so there is still a great reliance on the soil moisture evolution predicted by land surface models to obtain profile soil moisture information. Therefore, data assimilation techniques have been used to constrain root zone moisture estimates using satellite observations of near surface soil moisture (e.g. Albergel et al., 2008; Walker and Houser, 2001).

Amongst other things, land surface models (LSMs) are used to provide boundary conditions to weather and climate models, representing the land surface feedbacks to the atmosphere. Consequently, coupled land surface-atmosphere schemes must be able to predict the energy, water, and carbon exchanges, with explicit representation of vegetation and soil types. The LSMs generally

* Corresponding author. Tel.: +61 3990 54957; fax: +61 3990 54944.
E-mail address: Ranmalee.Bandara@monash.edu (R. Bandara).

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require meteorological data (temperature, precipitation, radiation and so on) and parameters of vegetation and soil characteristics as inputs (Abramowitz et al., 2007). However, soil moisture estimates using land surface models typically suffer from physical parameterisation based on low-resolution and/or erroneous soil property information (Grayson et al., 2006). Soil hydraulic parameters are either measured in situ or in a laboratory as point measurements. Consequently, it is impractical to use this approach to derive detailed information on spatial variability of the soil properties due to the time consuming nature of the tests and the expenses involved (Steele-Dunne et al., 2010). Hence, pedotransfer functions (empirical equations) are typically used to describe the relationship between the required soil hydraulic properties and easily measurable soil properties such as soil texture (Wösten, 1997; Wösten et al., 2001). Extrapolation over large areas yields crude estimates of soil hydraulic properties with large standard deviations (Vereecken et al., 1989, 1990), the accuracy of which deteriorates with the extent of the extrapolation, and thus adversely affects the accuracy of the model simulations. The origin of most global and local soil property maps is the Food and Agricultural Organization of the United Nations (FAO) soil texture map, known as the "World Soil Classification" (Latham, 1981), with the soil hydraulic properties estimated from look-up-tables for 'typical' soil types (e.g.: Clapp and Hornberger, 1978; Rawls et al., 1982). Yet, soils are a heterogeneous resource that changes on the scale of centimeters, and so hydraulic parameter estimates from a typical soil type have large deviations from reality.

Satellite based remote sensing is able to supply time series information of surface soil moisture data with 2–3 day repeat intervals over wide areas. However, given that there are several satellites orbiting the earth that provide soil moisture information, it would be possible to obtain daily moisture time series by combing these different products. Such data can potentially be used to estimate the hydraulic properties of the soil profile, through model calibration of observed and predicted surface soil moisture content. However, only a few studies have attempted to exploit such an approach. One of the earliest, perhaps the first, to estimate the soil hydraulic parameters from passive microwave measurements and atmospheric forcing data was by Camillo et al. (1986). In their study, a soil physics model was used to solve the heat and moisture flux equations in the soil profile, and a microwave emission model used to predict the soil brightness temperature. The model hydraulic parameters were then varied until the simulated soil brightness temperature agreed with the remotely sensed measurements from a dual-polarized L-band radiometer. However, the experiment was conducted within a time-frame of only 3 days on three artificially modified plots, and did not capture the full wetting and drying cycle of the soils. Santanello et al. (2007) undertook a similar study using a 6-week extended dry down period immediately following a rainfall event, and concluded that better performance can be expected when data during and immediately following a rainfall event are used. Harrison et al. (2012) extended the case study of Santanello et al. (2007) to include uncertainty estimation of soil hydraulic properties, concluding that remotes sensing estimates of soil moisture can lead to improved characterization of the uncertainties in land surface modelling. One major difference between the above studies and the work presented in this paper is, the soil hydraulic parameters are retrieved directly as opposed to inferring from the particle size distribution. More recently, a genetic algorithm was used by Ines and Mohanty (2008) to identify the soil water retention and hydraulic conductivity functions, through the inversion of a soil–water–atmosphere–plant (SWAP) model using observed near-surface soil moisture as a search criterion. Their study focused on three hydrological cases, a homogeneous column of soil under free-drainage, a homogeneous column of soil with a shallow water table, and a heterogeneous soil column under free-drainage. This study found that the soil hydraulic properties for only the surface layer could be identified for the heterogeneous soil column. The methodology was also tested with laboratory measured soil moisture, matric potential and hydraulic conductivity data, demonstrating that an effective homogeneous soil unit may fail to accurately represent a highly heterogeneous soil profile. The point-scale study of Ines and Mohanty (2009) was then tested for large-scale parameter estimation using soil moisture data from airborne remote sensing. An important observation of this study was that any uncertainties in the remotely sensed data at the retrieval, calibration or geoprojection stages can propagate directly to the derived soil hydraulic parameters at the pixel-scale. However, they have only focused on homogeneous columns of soil in all their work, and therefore have not explored the possibility of retrieving hydraulic parameters for a heterogeneous soil.

There has also been a recent synthetic study by Montzka et al. (2011), which explored the impact of the temporal sampling rate on the ability to correct model states and estimate soil hydraulic parameters. They used the method of sequential data assimilation with a one-dimensional mechanistic soil water model on four different homogenous soil types. Consequently, their study did not encompass heterogeneous soils, meaning that they did not investigate the capability of retrieving the soil hydraulic parameters for both the surface and root zone of the soil profile simultaneously, using surface observations. However, they did demonstrate that the 3-day repeat period of the Soil Moisture and Ocean Salinity (SMOS) mission is suitable for correcting model simulation biases that result from false parameterization, thus reducing the uncertainty of soil hydraulic parameters. This is important, as it confirms the potential to retrieve soil hydraulic parameters using remotely sensed surface soil moisture information from satellite missions such as SMOS.

This paper develops a methodology, and determines the level of accuracy that can be expected, for soil hydraulic property estimation from heterogeneous soil profiles using near surface soil moisture observations, such as those that are available from satellites. Moreover, this paper identifies the meteorological conditions under which the soil hydraulic parameters are best retrieved, so as to optimize the computational efficiency when applied to large areas. First, the most sensitive soil hydraulic parameters are identified through a series of single parameter retrieval experiments, followed by testing under a range of soil types, and application to multi-parameter retrieval for duplex soil profiles. This study uses the Joint UK Land Environment Simulator (JULES) as the multi-layered land surface model (Best et al., 2011; Clark and Harris, 2009; Clark et al., 2011), and an optimization method that is based on the complex, collective behavior of individuals in decentralized, self-organizing systems, falling within the category of 'swarm intelligence' (Kennedy and Eberhart, 1995).

2. Site and data description

The work presented in this paper focuses on the Y3 site (34.6208S, 146.4239E) located near Yanco, New South Wales, Australia. This is one of the OzNet soil moisture monitoring sites (Smith et al., 2012); http://www.oznet.org.au/, and is co-located with the Bureau of Meteorology (BoM) automatic weather station (AWS) 074037. The soil is of duplex nature, with the first layer (horizon A) being approximately 0.30 m deep. The site has an elevation of 164.7 m above mean sea level with the dominant surface soil type being silty sand (Australian Bureau of Rural Science). The surface (0–8 cm) soil moisture has been measured every 5 s and averaged to 30 min intervals while the surface soil temperature (4 cm) has been measured at 6 min intervals. The precipitation was measured by the use of a tipping bucket rain gauge, with the cumulative rainfall recorded every 6 min (Smith et al., 2012).

This work focuses on the year 2003, which was a year where the soil moisture ranged from extremely dry (0.04 m^3/m^3 at the surface and 0.12 m^3/m^3 at the root zone) to extremely wet (0.45 m^3/m^3 at the surface and 0.38 m^3/m^3 at the root zone) conditions as shown in Fig. 1. Daily rainfall totals were a maximum of 120 mm for the year 2003. The half-hourly atmospheric forcing data needed to drive the land surface model were derived from the Yanco AWS data (Siriwardena et al., 2003). Initial conditions for the surface layer, corresponding to both the truth run and optimization process, were derived from in situ observations of soil moisture and temperature. The texture information for the selected soil type was obtained from the default Food and Agriculture Organization of the United Nations' (FAO) soil texture map as well as from site observed particle size distribution data, and the soil properties used as input to JULES were calculated using the pedo-transfer functions of Cosby et al. (1984).

To facilitate the investigation of meteorological conditions and their impact on soil hydraulic property retrieval, five different weather scenarios were selected as shown in Fig. 1, including short dry-down (SDD), short dry (SD), short wet-up (SWU), short wet (SW), and year-long (LT) periods. The methodology was tested for four soil profiles as; (a) homogeneous column of sand, (b) horizon A with loamy/silty sand and horizon B with clay, (c) same as (b) but with the horizons inter-changed and, (d) homogeneous column of clay. The soil hydraulic parameters estimated from Cosby et al. (1984) pedo-transfer functions using the particle size distribution data corresponding to each chosen soil were termed as 'true' parameters. The reason for using field observed meteorological and initial surface soil moisture conditions to create the synthetic time series of "truth" soil moisture is to make this data as close as possible to typical field observations, but without any model biases. To obtain initial root zone soil state values throughout the profile from the surface observations, the LSM model was spun-up to equilibrium.

3. Model description

The land surface model of this study is the JULES multi-layered land surface model (Best et al., 2011; Clark and Harris, 2009; Clark et al., 2011). It was used to simulate time-series soil moisture corresponding to pre-determined soil hydraulic parameters, which provide the 'true' parameter values and corresponding surface and root zone soil moisture time-series. Soil hydraulic parameter(s) were then perturbed to represent the range of uncertainty in one or more parameters, yielding what has been termed here as the 'test' parameters and time-series soil moisture. Next the particle swarm optimizer was used to 'retrieve' the perturbed parameter(s) by comparing the predicted and 'true' surface soil moisture. The 'retrieved' parameter(s) are then validated against the 'true' parameter value(s), and the root zone soil moisture corresponding to the 'retrieved' parameter(s) validated against the 'true' soil moisture of the root zone. A schematic of the methodology is shown in Fig. 2.

3.1. Joint UK Land Environment Simulator – JULES

The Joint UK Land Environment Simulator (JULES) is a process based land surface model (LSM) that simulates the fluxes of carbon, water, energy and momentum between the land surface and the atmosphere, and is a derivative of the Met Office Surface Exchange Scheme (MOSES) (Cox et al., 1999). It can function either as a stand-alone model or coupled to a global circulation model. In a previous study, Bandara et al. (2011) assessed the performance of JULES and recommended it as a suitable model for this type of study.

The JULES LSM consists of four sub-models: soil, snow, vegetation and radiation (Best et al., 2011; Clark and Harris, 2009; Clark et al., 2011). Of these, the focus is on the soil sub-model and the simulation of soil moisture. By default, JULES uses four soil layers of 0.10 m, 0.25 m, 0.65 m and 2.0 m thickness, resulting in an overall soil depth of 3.0 m. However, both the number of layers and their thickness can be varied by the user, with the parameters and initial state values specified for each of the soil layers. Richard's equation and the Brooks and Corey (1964) constitutive relationships are used in the calculation of soil moisture. JULES has a tiled model of sub-grid heterogeneity with nine surface types available; broad leaf trees, needle leaf trees, C3 (temperate) grass, C4 (tropical) grass, shrubs, urban, inland water, bare soil and ice. However, the work presented here is for a single one-dimensional

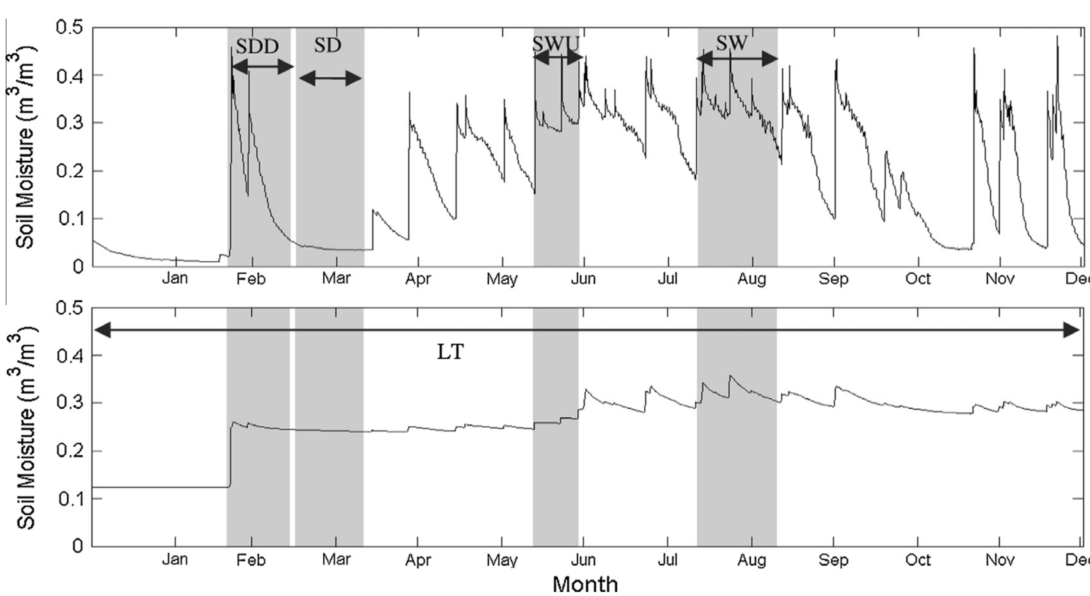

Fig. 1. Simulated surface (top) and root zone (bottom) soil moisture, the shaded areas from left to right represent, the short dry-down (SDD), the short dry (SD), the short wet-up (SWU), the short wet period (SW) and, long term (LT) periods.

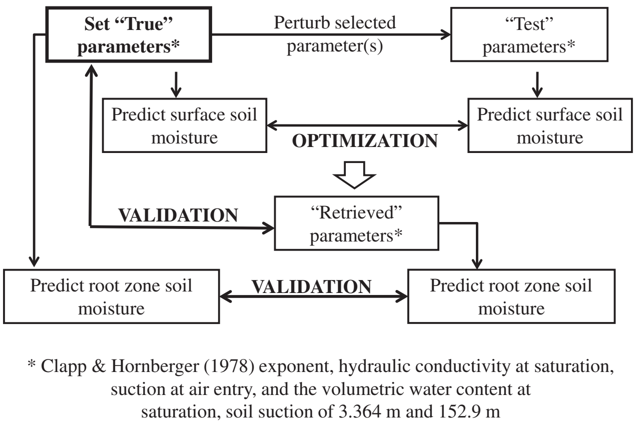

Fig. 2. Schematic of the parameter retrieval process.

soil column with the surface assumed to be bare soil. This assumption does not impact the synthetic results here. Moreover, the results are expected to be representative of those from application in low-to-moderate vegetation conditions, as the vegetation would only have a small impact on the evapotranspiration and the depth in the soil from which moisture is extracted by roots.

The soil hydraulic parameters that are retrieved in this paper include; (a) Clapp and Hornberger exponent, (b) hydraulic conductivity at saturation, (c) soil matric suction at air entry, (d) volumetric fraction of soil moisture at saturation, (e) volumetric fraction of soil moisture at the critical point, equivalent to a soil suction of 3.364 m and, (f) volumetric fraction of soil moisture at wilting point, assumed to be for a soil suction of 152.9 m; see Table 1.

3.2. Particle Swarm Optimization – PSO

Particle Swarm Optimization (PSO) is an algorithm based on the complex, collective behavior of individuals in decentralized, self-organizing systems, and are created through a population of individuals that interact both with each other and with the community (Kennedy and Eberhart, 1995). Swarms of birds, colonies of ants, and schools of fish are some of the examples that can be identified from nature. One advantage of Particle Swarm Optimization (PSO) is that it is easy to understand and to implement (Kennedy and Eberhart, 1995). The main feature is that it is less susceptible to getting trapped in a local minimum since it is population-based, and it has the capability to control the balance between the local and global search space (Engelbrecht, 2005b). It has been implemented successfully in a diverse range of applications such as calibration of water and energy balance models (Scheerlinck et al., 2009), multi-machine power-system stabilizers (Abido, 2002), practical engineering designs (Hu et al., 2003), and structural designs (Perez and Behdinan, 2007).

Table 1
Overview of the six soil hydraulic parameters, along with their respective symbol, descriptive name, and unit where applicable.

Parameter (shortened name)	Parameter name and unit
b	Clapp and Hornberger exponent (–)
K_s	Hydraulic conductivity at saturation (mm/s)
ψ_a	Soil matric suction at air entry (m)
θ_s	Volumetric fraction of soil moisture at saturation (m^3/m^3)
θ_c	Volumetric fraction of soil moisture at critical point (for a soil suction of 3.364 m) (m^3/m^3)
θ_w	Volumetric fraction of soil moisture at wilting point (for a soil suction of 152.9 m) (m^3/m^3)

In the context of PSO, individuals are referred to as 'particles' and are flown through a hyper-dimensional search space where changes to the particle's position are based on the social-psychological tendency of the individual to mimic the success of others (Engelbrecht, 2005b). Any changes to the position of particles within the search space are thus influenced by the experience or knowledge of its neighbors as well its' own. The algorithm consists of three parts; (a) the momentum that states that the velocity of the 'swarm' cannot change abruptly, (b) the 'cognitive' or personal part (c_1) that indicates the particle learns from its own flying experience and fitness and, (c) the 'social' part (c_2) that represents the cooperation with the other particles or the learning from the flying experience of the group (Kennedy and Eberhart, 1995). However, one disadvantage of updating the velocity of the 'swarm' of the algorithm is that it may become too high and cause particles to pass 'good' solutions or vice versa, such that the search space is explored inadequately. To overcome this problem, Shi and Eberhart (1998) found that the use of an additional parameter, termed as 'inertia weight', could be used to control the velocity. The work presented here uses the PSO code from Scheerlinck et al. (2009).

As a first step of applying PSO, the 'best' parameters for driving the swarm in PSO need to be identified and specified. This is essential because the algorithm uses four parameters, three inherent parameters, and the population size to define the behavior of the swarm. The first factor considered in this work was the size of the swarm, as larger swarms need a higher number of iterations to converge compared to smaller swarms, with very small swarms not yielding good solutions. Eberhart and Shi (2000) showed that a population size of 30 is an adequate sample size. This was also adopted by Trelea (2003), Engelbrecht (2005b), Scheerlinck et al. (2009) and others. Hence, a population size of 30 particles was chosen for this study.

Shi and Eberhart (1998) suggest that when w (the inertia weight) is less than 1, the PSO is able to find the global minimum quite fast because the PSO tends to act like a local search algorithm under this scenario and focuses on an acceptable solution within the initial search space. When $w \geqslant 1$, the velocities of the swarm increase with time, the swarm diverges, and the particles fail to change direction towards regions with potential minima (Engelbrecht, 2005a). Moreover, Engelbrecht (2005a) states that $c_1 > c_2$ is more beneficial when applied to multimodal problems as lower values of c_1 and c_2 yield smooth particle trajectories. The windows that best fit the work presented in this paper were identified from existing literature, as discussed above, and parameter w was varied between 0.2 and 0.5, c_1 between 1 and 2, and c_2 between 0.8 and 2, in steps of 0.1. From trial and error it was found that the best combination of parameters for this problem was $w = 0.4$, $c_1 = 1.4$ and $c_2 = 1.3$.

The objective function used by PSO in this paper is the root mean square error (RMSE). It is necessary to restrict the parameter(s) within the parameter space during the optimization process so that it does not attempt to move beyond physical values during the application of the algorithm. This restriction is achieved through specification of the model parameter range. To further constrain the parameter from jumping to either end of the parameter space, an extra penalty was added to the RMSE calculated between the true and simulated soil moisture. The penalty was such that the parameter to be retrieved was given an initial approximate or best-guess value, with a variation of three times the standard deviation of that parameter, thereby making the parameter space somewhat smaller and directing the optimization algorithm away from boundary values.

4. Sensitivity studies

By decreasing the number of soil parameters to be retrieved, the complexity of the parameter space is reduced, thereby making the optimization more reliable, meaningful and speedy. It was therefore necessary to identify those soil parameters that have the most influence over the moisture simulation, through sensitivity studies. Consequently, pre-selected soil parameter variables were perturbed across a physically meaningful range and the corresponding output assessed for the impact. The JULES model simulates a variety of states and fluxes including soil temperature, soil moisture, soil evaporation, transpiration and so on. Since the focus of this study is on soil moisture, other data will not be discussed further in the study. As not all of the soil parameters contribute equally towards moisture simulation, the importance of some might be under-represented by the results presented here.

Sensitivity is typically defined as the relative magnitude of changes in the model response as a function of relative changes in the values of model input parameters (Nearing et al., 1990). Thus, this study uses a single-value sensitivity index that represents a relative normalized change in output to a normalized change in input. The higher the absolute value of the index, the greater the impact an input parameter has on a particular output. An index of 1.0 indicates that the output responds to the same degree as the tested input is perturbed around an average range; a negative value indicates that the input and output are inversely related (Al-Abed and Whiteley, 2002; Nearing et al., 1990; Walker, 1996). The sensitivity index (S) is defined as

$$S = \left(\frac{O_2 - O_1}{I_2 - I_1}\right)\frac{I_{avg}}{O_{avg}} \tag{1}$$

where I_1 and I_2 are the smallest and highest input values tested for a given parameter, I_{avg} is the average of I_1 and I_2, O_1 and O_2 are the model output values corresponding to I_1 and I_2, and O_{avg} is the model output value corresponding to I_{avg} (approximately the average of O_1 and O_2). The sensitivity index is calculated for each model time step and as it is both dimensionless and independent of the magnitude of the input and output, its value can be used to compare the sensitivity of the model to different variables (Baffaut et al., 1996).

For each parameter tested for sensitivity, three soil moisture time series have been established using the published soil parameter data and the accompanying standard deviations given in Clapp and Hornberger (1978). The first time series was generated using the parameter value minus the standard deviation, the second corresponds to the parameter value itself, and the third time series was from the parameter value plus the standard deviation. These three soil moisture time series were taken as the values of O_1, O_{avg} and O_2 respectively, with the parameter sensitivity index calculated as a time series with a single value of S at each instance of time. Fig. 3 shows the surface and root zone sensitivity indices for each of the eight soil parameters used in JULES. A common scale ranging from -1 to 2 has been used to facilitate easy comparison, and hence some parameters that are more sensitive to soil moisture simulation exceed these ranges. Table 1 gives an overview of the six soil parameters that have been identified as showing the highest impact on soil moisture simulation.

The sensitivity analysis results in Fig. 3 show that during the extreme dry period at the beginning of the year, the LSM is sensitive only to changes in the volumetric fraction of soil moisture at critical point while being insensitive to changes in all other parameters. Under the wet conditions observed during the months of June to September, the volumetric fraction of soil moisture at saturation displays a near-zero trend which is due to the fact that at the point of near-saturation, changes to the parameter will not affect the soil moisture simulation. For the same period, the volumetric fraction of soil moisture at saturation and the matric potential at air entry display changes according to the wetness and dryness of the soil as air entry is not possible near saturation. These results imply that the significance of these soil parameters is dependent on the moisture state, and that their response is correlated to the current state. However, the purpose of this sensitivity analysis was to identify the soil parameters that most influence the soil moisture simulation. Hence, of the eight soil parameters that have an impact on soil moisture, the volumetric fraction of soil moisture at critical point and at saturation, as well as the Clapp and Hornberger exponent, show the highest sensitivity. The hydraulic conductivity at saturation, the volumetric fraction of soil moisture at wilting point and the soil matric suction at air entry, show much less, but none-the-less important, sensitivity. In contrast, the dry heat capacity and dry thermal conductivity show minimal sensitivity and so are eliminated from the list of retrievable parameters.

5. Parameter retrieval

The schematic of the parameter retrieval process is shown in Fig. 2, and was briefly discussed already under Section 3. This study proposes the retrieval of the root zone soil hydraulic parameters from surface soil moisture observations alone, and hence it was necessary to correctly specify the initial states for both the surface and root zone. Therefore the observed near-surface soil moisture and soil temperature were used as initial conditions for the surface layer while the results corresponding from the spin-up were used for the root zone.

As the first step of testing the proposed methodology, single parameters were retrieved by perturbing parameters one at a time, representing the uncertainty in published soil hydraulic parameter data. The inclusion of single-parameter-at-a-time retrieval was to investigate the complete range of optimization possibilities, from a single parameter (one for each soil type) right through to all six parameters (for each soil type), thus accounting for complexity of search space and parameter cross-correlation identified by Vrugt et al. (2003). Using the predicted soil moisture resulting from perturbed parameters, together with the surface soil moisture observations time series, the original set of 'true' parameters throughout the soil column are retrieved. The optimized parameters have the prefix 'retrieved' throughout the paper.

The second step was to jointly retrieve all six parameters, as opposed to individually. Three methods were used for this; (a) all six parameters retrieved simultaneously, (b) sequential retrieval of two parameters at one time and, (c) sequential retrieval of three parameters at one time. In the sequential retrieval, (b) and (c), the combinations were from the most sensitive to the least sensitive parameters.

All four soil type combinations were tested under the five different meteorological periods identified. The corresponding RMSE between the soil moisture using the true and retrieved parameters were calculated along with the Nash–Sutcliffe model efficiency coefficient (Nash and Sutcliffe, 1970). The Nash–Sutcliffe coefficient E can range from $-\infty$ to 1, with a perfect match between the modelled simulation and observation resulting in a value of $E = 1$. When $E = 0$, the model predications are as accurate as the mean of the observed data, whilst for values of $E < 0$ the observed mean is a better predictor than the model.

6. Results and discussion

6.1. Retrieval of one parameter at a time

The first objective of the study was to identify the meteorological condition under which the selected hydraulic property can

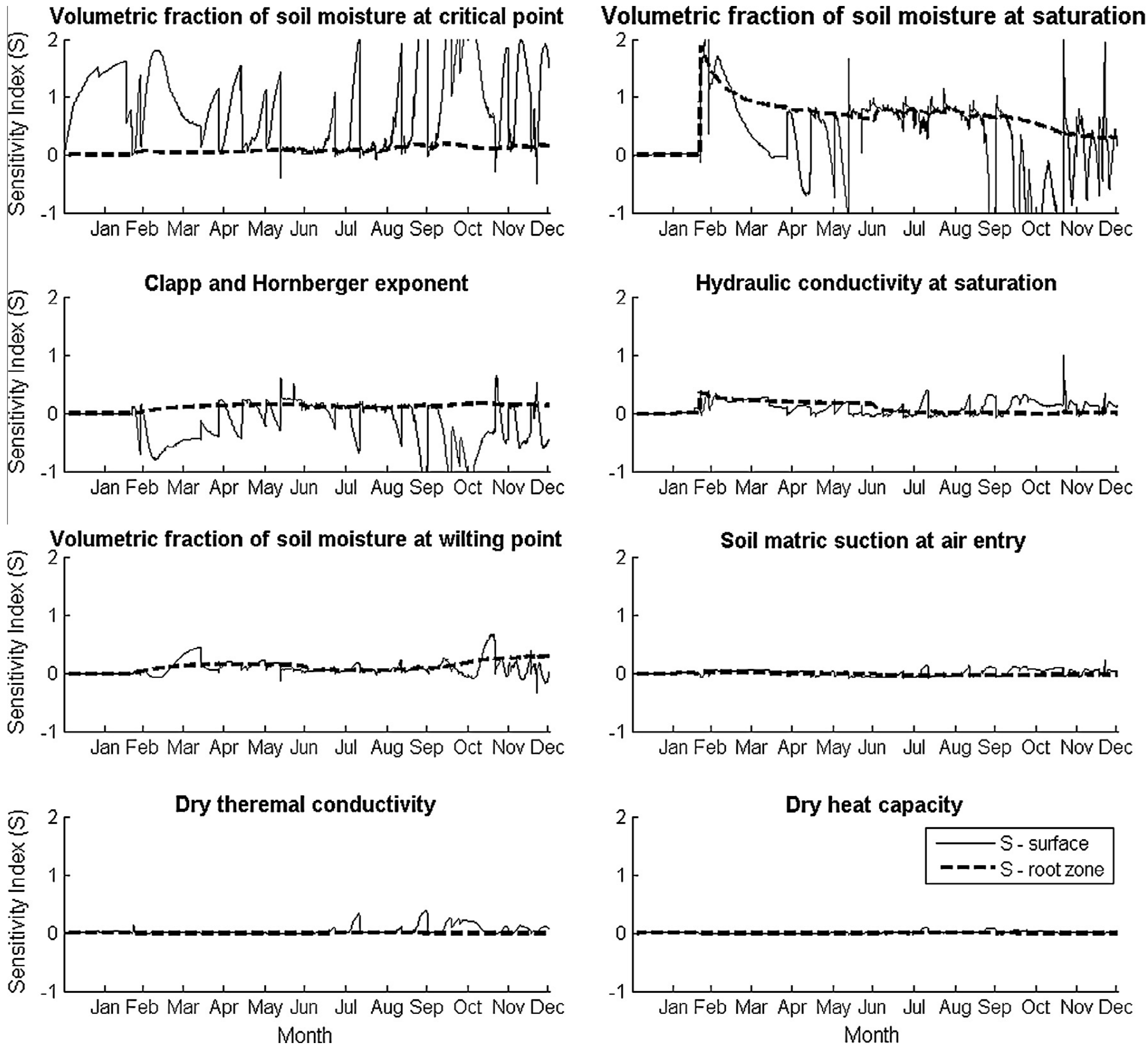

Fig. 3. The sensitivity index (*S*) plotted against time for each soil parameter.

best be retrieved. The RMSEs calculated under the different meteorological conditions (Table 2) and the corresponding Nash–Sutcliffe model efficiency coefficients (Table 3) were compared, together with the 'retrieved' and 'true' parameter values, as summarized in Table 4. It is immediately clear when comparing the retrieval efficiency of the four soil types, that the retrieval was not able to adequately optimize the parameters of the clay/sand combination, apart from the 12-month long (LT) scenario. Conversely, the highest skill for soil parameter retrieval across all meteorologic conditions was for the homogeneous column of clay when compared to the other soil types. The results are found to be similar for the homogeneous column of sand and the silty sand/clay combination.

It is also observed that some parameters are better retrieved under different meteorologic conditions for different soil types. For example, the volumetric fraction of soil moisture at critical point could be retrieved under all meteorological conditions for a homogenous column of clay, which is opposite to the mixed soil column comprising of clay/sand, where retrieval was only possible during the long term period. For the mixed column of silty loam/clay, the retrieval worked well only for the long term and short dry-down periods, while all meteorological conditions apart from the short dry period showed good results for the homogeneous column of sand.

When there is a homogeneous column of soil, the parameter space is smaller and less complicated, compared to a mixed soil column. Because of this, the retrieval of parameters is comparatively better under all the meteorological conditions tested. In this case, it is observed that the non-complexity of the parameter space plays a more significant role than the inherent soil characteristics. Sandy soil is swift to react to changes and during the short-dry season, quickly becomes de-coupled between the surface and root zone, thereby influencing the retrieval capability of the selected soil hydraulic parameters. For the mixed column of clay/sand (where horizon A comprises of a 0.30 m of clay), the layer of fine clay on the upper horizon takes a long time to react to any changes near the surface, thereby constraining any changes that occur to the sandy soil on the lower horizon. Hence, the longer the time-series, the more time there is for the top soil to react to changes, and subsequent changes to the root zone. Silty loam can have up to 29% clay and therefore takes more time to react to changes compared to a sandy soil, but considerably less time compared to a clay soil. Hence, soil parameter retrieval could only be achieved with the silty loam/clay column during the longest time-series. The drying-down period was selected after a very significant rainfall of about 120 mm/day following an extremely dry period. This wetting event has contributed to the models capability for hydraulic parameter retrieval within the short dry-down period.

Table 2
The root mean square error (RMSE) between surface and root-zone soil moisture using 'retrieved' and 'true' soil hydraulic parameters when retrieving only one parameter at a time. Results are for a silty sand/clay soil type under the five different meteorological conditions tested. The sequence of parameters is listed from the most sensitive to the least sensitive.

Parameter	RMSE (m^3/m^3)									
	Short wet-up period		Short wet period		Short dry-down period		Short dry period		Long term period	
	Surface	Root zone	Surface	Root zone	Surface	Root zone	Surface	Root zone	Surface	Root zone
θ_c	1.65e−05	5.80e−06	2.07e−09	1.15e−10	0.0000	0.0000	0.0000	0.0000	4.00e−05	1.15e−05
θ_s	0.0204	0.0300	0.0156	0.0441	0.0015	0.0210	0.0002	0.0124	0.0029	0.0019
b	0.0006	0.0004	0.0002	6.60e−05	0.0003	0.0005	8.48e−05	8.66e−05	0.0004	0.0002
K_s	0.0027	0.0055	0.0000	0.0000	0.0045	0.0179	9.04e−05	0.0008	0.0104	0.0034
θ_w	3.08e−09	1.94e−10	2.07e−09	1.15e−10	1.41e−09	9.84e−11	0.0000	0.0000	1.64e−07	3.25e−08
ψ_a	0.0000	0.0000	3.24e−05	1.43e−05	2.69e−07	5.52e−07	2.58e−05	0.0001	0.0024	0.0017

Table 3
As for Table 2 but with Nash–Sutcliffe model efficiency coefficients (E).

Parameter	Nash–Sutcliffe model efficiency coefficients (E)									
	Short wet-up period		Short wet period		Short dry-down period		Short dry period		Long term period	
	Surface	Root zone	Surface	Root zone	Surface	Root zone	Surface	Root zone	Surface	Root zone
θ_c	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
θ_s	0.8642	0.9899	0.9395	0.4663	0.9992	0.7535	0.9999	0.4729	0.9985	0.9964
b	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	1.0000	0.9998	0.9999	0.9999
K_s	0.9977	0.9881	1.0000	1.0000	0.9930	0.7775	1.0000	0.9999	0.9803	0.9817
θ_w	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
ψ_a	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	0.9999	0.9989	0.9924

Table 4
Matrix showing the cases where individual parameter retrieval was successful for the different soil types and meteorological conditions tested. The solid circle shows instances where the parameter was retrieved within 5% of the 'true' value, E is greater than 0.9, and the RMSE is less than 0.009 m^3/m^3; the open circle shows that parameter retrieval was attempted but was unsuccessful.

Parameter	Sand					Silty sand/clay					Clay/sand					Clay				
	SWU	SW	SDD	SD	LT	SWU	SW	SDD	SD	LT	SWU	SW	SDD	SD	LT	SWU	SW	SDD	SD	LT
θ_c	●	●	●	○	●	○	○	●	○	●	○	○	○	○	●	●	●	●	●	●
θ_s	●	●	●	●	●	○	●	●	●	●	○	○	○	●	●	●	●	○	○	○
b	○	○	●	●	●	●	●	●	●	●	○	○	○	○	●	●	●	●	●	●
K_s	●	○	○	●	●	○	●	○	●	●	●	○	○	○	●	●	●	●	●	●
θ_w	○	○	○	○	○	○	○	○	○	●	○	○	○	○	●	○	○	○	○	●
ψ_a	●	●	●	●	●	●	●	●	●	○	○	○	●	○	●	●	●	●	●	●

The volumetric fraction of water at wilting point is not retrieved so readily as the other soil parameters. In fact, it was not possible to retrieve this parameter for the homogeneous column of sand at all, with retrieval for the other soil types only achieved under the long term condition. The Nash–Sutcliffe model efficiency parameter for the volumetric fraction of water at wilting point was unity in most cases, indicating that the simulation and 'true' observations of soil moisture are a perfect match. Since this parameter is mostly important in the calculation of leaf photosynthesis, the bare soil assumption of this study is likely to have impacted any conclusions in relation to this parameter.

While the methodology was tested for four soil types encompassing all spectra of soil texture, the site of interest mainly consists of silty loam covering a deeper layer of clay. In addition, it was noted from Table 4 that the 12-month period yielded the best results for all soil types across the range of tested meteorological conditions. Similarly, Table 5 focuses on the 'true' and 'retrieved' parameter values for horizons A and B for the silty sand/clay soil type combination shown in Tables 2 and 3 under the long term scenario. From Table 5, it is seen that the Clapp and Hornberger coefficient and the volumetric fraction of soil moisture at critical point are retrieved to an accuracy of 99.9%, whereas the other parameters, apart from the suction at air entry, are within 5% of the 'true' values. The RMSE for the volumetric fraction of soil moisture at wilting point is close to zero with a Nash–Sutcliffe of unity, indicating a perfect retrieval. However, the bare soil of this study is likely the cause of model insensitivity to changes in the parameter (as per the summary in Table 4).

6.2. Retrieval of multiple parameters at one time

Results corresponding to the "simultaneous" retrieval of all six parameters in Table 6 are based on three different approaches. The first approach retrieves the six parameters at once; the second is the sequential retrieval of two parameters at a time, while the third approach is the sequential retrieval of three parameters at a

Table 5
The 'true' and 'retrieved' soil parameter values for horizons A (HA – silty sand) and B (HB – clay) for the long term period with single parameter retrieval.

Parameter	'True' parameter values		'Retrieved' parameter values	
	HA	HB	HA	HB
θ_c	0.215	0.384	0.2149	0.3998
θ_s	0.419	0.457	0.4238	0.4597
b	4.65	13.57	4.648	13.571
K_s	0.0081	0.0011	0.0090	0.0015
θ_w	0.095	0.290	0.1000	0.2999
ψ_a	0.153	0.313	0.1700	0.3858

Table 6
Retrieved soil parameters (top) and associated RMSE in derived soil moisture (bottom) under the long term period for three different multi-parameter retrieval scenarios with simultaneous and sequential retrieval; horizon A (HA – silty sand) and B (HB – clay).

Parameter	Simultaneous retrieval of of all 6 parameters		Sequential retrieval of 2 parameters at a time		Sequential retrieval 3 of parameters at a time	
	HA	HB	HA	HB	HA	HB
θ_c	0.1431	0.2542	0.2086	0.2558	0.2231	0.2786
θ_s	0.4698	0.4316	0.4130	0.4579	0.4158	0.4587
b	5.146	13.234	4.752	13.289	4.711	13.304
K_s	0.0033	0.0006	0.0086	0.0465	0.0072	0.0630
θ_w	0.0801	0.2423	0.1784	0.2210	0.1152	0.1341
ψ_a	0.0333	0.0722	0.0445	0.0126	0.1528	0.0760
	Surface	Root zone	Surface	Root zone	Surface	Root zone
Moisture (m^3/m^3)	0.0445	0.0126	0.0236	0.0153	0.0153	0.0184

time. In all three methodologies, the surface and root zone hydraulic parameters corresponding to the entire soil profile have been retrieved simultaneously. Fig. 4 shows the soil moisture time series analogous to Table 6, where the soil moisture was simulated from the 'true' and 'retrieved' parameters.

It is observed that Fig. 4c shows the best match between the surface layer soil moisture time series using the 'true' and 'retrieved' parameters, while Fig. 4a has the 'best' match for the root zone, when compared to the other scenarios. The retrieved parameters of Horizon A (HA) for the first scenario do not match closely with the 'true' values, resulting in a relatively high RMSE value (almost 50% more) when compared to the second and third approaches. The parameters for HA are best retrieved under the third method, having the lowest RMSE of 0.015 m^3/m^3, with the second approach performing slightly less well with a RMSE of 0.023 m^3/m^3. This is again due to the fact that the parameter space is made comparatively more complex when soil hydraulic parameters are being retrieved for two soil horizons. However, for the soil hydraulic parameters for Horizon B (HB), the RMSEs are opposite to HA. The lowest RMSE of 0.012 m^3/m^3 corresponds to the first scenario (almost 50% higher) while the highest value is given by the sequential retrieval of three parameters (about 70% higher). It is also observed that the RMSEs corresponding to all three scenarios differ by a maximum value of 0.006 m^3/m^3.

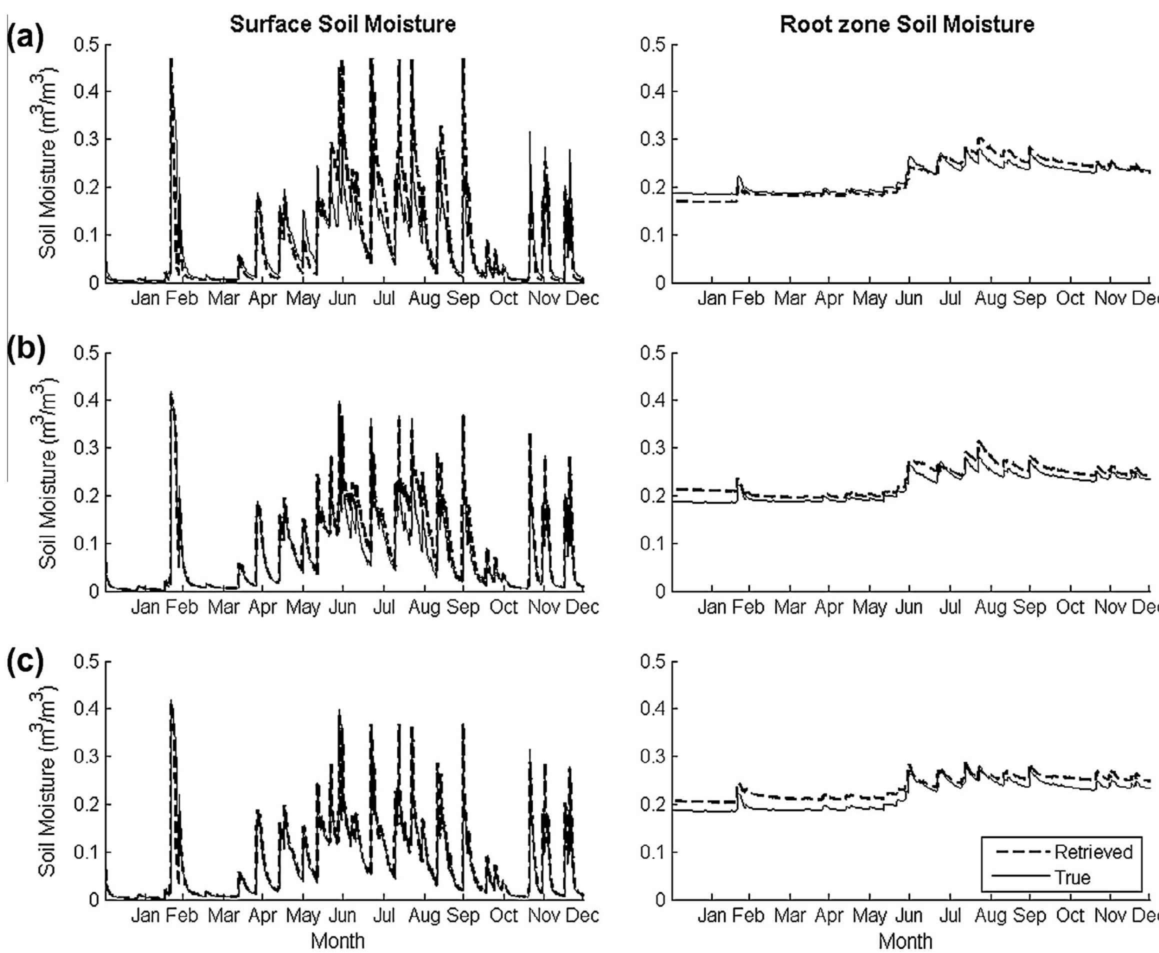

Fig. 4. The surface (left) and root-zone (right) soil moisture for the 12-month period using 'true' and 'retrieved' parameters: (a) simultaneous retrieval of all 6 parameters, (b) sequential retrieval of 2 parameters at a time, and (c) sequential retrieval of 3 parameters at a time.

The Clapp and Hornberger coefficient and the soil moisture at saturation have consistently been retrieved within an accuracy of 5% of the ‘true’ values under all three scenarios. Hence, it can be stated that these parameters can be retrieved from any of the three approaches. The root zone soil moisture is not as dynamic as the surface layer and thus, unless the most sensitive parameters alter significantly, the changes are not captured. If the true root zone soil moisture is available and is used in the soil hydraulic parameter retrieval process, it will allow a better match for the retrieved parameters corresponding to the root zone. However, this is not typically the case, and since only the top 5 cm (surface) soil moisture is observed by satellite remote sensing, this study has investigated the alternative method of obtaining the soil hydraulic parameters of the root zone using only the surface data.

7. Conclusions

The soil parameters most sensitive to the soil moisture simulation using the JULES model were identified as: (a) the volumetric fraction of soil moisture at the ‘critical point’, (b) the volumetric soil moisture at saturation, (c) Clapp and Hornberger exponent, (d) the hydraulic conductivity at saturation, (e) the soil matric suction at air entry, and (f) the volumetric fraction of soil moisture at wilting point, in this order of priority. A methodology was developed and tested for retrieving these parameters based on surface soil moisture observations, as would be available from remote sensing, for a range of different meteorological conditions; (a) short dry-down, (b) short dry, (c) short wet-up, (d) short wet and, (e) 12-month periods, with the objective of identifying the most suitable meteorological condition for the retrieval. The overall observation was that soil hydraulic parameters were best retrieved when using a12-month period of observation, which includes several wetting and drying cycles. It was also observed that parameters are best retrieved when there is a higher percentage of clay in the soil column as opposed to a more sandy soil.

Different parameter combinations were tested for the simultaneous retrieval of two or more parameters, including all 6 parameters at the same time, and the 2 or 3 most sensitive parameters consecutively. It was found that parameters could not be retrieved with perfection using any of the three methods, despite the perfect input and simulation conditions of this twin study. However, some parameters were retrieved more closely than others, including the volumetric fraction of water at saturation and Clapp and Hornberger exponent. Irrespective, the RMSEs between the true soil moisture and that predicted when using the retrieved parameters were less than 0.02 m^3/m^3 for both surface and root zone, further demonstrating the poor sensitivity of the volumetric fraction of water at wilting point and the soil matric suction at air entry to soil moisture prediction. The best approach for retrieving all six soil hydraulic parameters for a duplex sand/clay soil type was found to be sequentially retrieving the three most sensitive parameters followed by the remaining three less sensitive parameters.

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